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A general formula for the Magnus expansion in terms of iterated integrals of right-nested commutators

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Abstract

We present a general expression for any term of the Magnus series as an iterated integral of a linear combination of independent right-nested commutators with given coefficients. The relation with the Malvenuto–Reutenauer Hopf algebra of permutations is also discussed.

1. Introduction

Given the linear differential equation

$$Y'(t) = A(t)Y(t), \qquad Y(0) = I, \tag{1}$$

where $A(t)$ is a $N \times N$ matrix, it is well known that $Y(t) = \exp\left(\int_0^t A(s)\,ds\right)$ is no longer the solution unless $[A(t_1), A(t_2)] = 0$ for arbitrary t_1, t_2, or at least $\left[\int_0^t A(s), A(t)\right] = 0$, where $[A, B] \equiv AB - BA$ denotes the usual commutator. One can still get an exponential approximation for the solution of (1), however, by applying a procedure proposed by Magnus [24]. In that case

$$Y(t) = \exp \Omega(t), \tag{2}$$

where Ω is now an infinite series

$$\Omega(t) = \sum_{k=1}^{\infty} \Omega_k(t), \qquad \text{with} \qquad \Omega_k(0) = 0, \tag{3}$$

whose terms are increasingly complex expressions involving time-ordered integrals of nested commutators of A evaluated at different times. It is the purpose of this work to provide a *general expression* for this series as iterated integrals of linear combinations of *independent* commutators.

In its original formulation [24], the Magnus expansion was established more generally as follows. Let $A(t)$ be a known function of t in the ring of all power series of the type

$$A(t) = \sum_{n=0}^{\infty} u_n t^n$$

and let $Y(t)$ be an unknown function satisfying the initial value problem (1). Then it is possible to express $Y(t)$ as (2), where $\Omega(t)$ is obtained by inserting (2) into (1) and solving the differential equation

$$\frac{d\Omega}{dt} = \sum_{n=0}^{\infty} \frac{B_n}{n!} \operatorname{ad}_\Omega^n A, \qquad \Omega(0) = 0. \tag{4}$$

by iteration. Here

$$\operatorname{ad}_\Omega^0 A = A, \qquad \operatorname{ad}_\Omega^{k+1} A = [\Omega, \operatorname{ad}_\Omega^k A], \qquad k \geqslant 0$$

and $\{B_j\}$ are Bernoulli numbers. This procedure leads to an infinite series for Ω,

$$\Omega(t) = \Omega_1(t) + \Omega_2(t) + \Omega_3(t) + \cdots$$

the first terms of which are

$$\Omega_1(t) = \int_0^t A(t_1)\,dt_1,$$

$$\Omega_2(t) = -\frac{1}{2}\int_0^t \left[\int_0^{t_1} A(t_2)\,dt_2, A(t_1)\right] dt_1$$

$$\Omega_3(t) = \frac{1}{12}\int_0^t \left[\int_0^{t_1} A(t_2)\,dt_2, \left[\int_0^{t_1} A(t_2)\,dt_2, A(t_1)\right]\right] dt_1$$

$$+ \frac{1}{4}\int_0^t \left[\int_0^{t_1} \left[\int_0^{t_2} A(t_3)\,dt_3, A(t_2)\right] dt_2, A(t_1)\right] dt_1 \tag{5}$$

and a more involved expression for Ω_4 (see e.g. [19]). It can be shown that one has convergence in a neighborhood of $t = 0$. By doing some algebra it is possible to write down explicitly at least the first Ω_k as linear combinations of iterated integrals of nested commutators of A evaluated at different times, but the complexity of this task increases steadily with k. For instance, working out the successive integrals appearing in Ω_3 as given by (5) we get

$$\Omega_3(t) = \frac{1}{6}\int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \left([A(t_1), [A(t_2), A(t_3)]] + [A(t_3), [A(t_2), A(t_1)]]\right), \tag{6}$$

whereas similar expressions for Ω_4 and Ω_5 have been presented in [29]. At any rate, this structure is especially favorable in practice when the differential equation evolves in a Lie group and the series is truncated: the approximation thus obtained still belongs to the same Lie group and thus shares with the exact solution relevant qualitative properties [10, 19].

Since the 1960s the Magnus expansion (often with different names) has been used to render analytical approximations in many different areas of science, ranging from nuclear, atomic and molecular physics to nuclear magnetic resonance, quantum electrodynamics, control theory, and also as a numerical integrator for differential equations in the realm of geometric numerical integration (see [10] for a review). Here the aim is to construct integration schemes that preserve the main qualitative features of the exact solution, such as its invariant quantities or the geometric structure [8, 17]. The convergence of the expansion is also an important feature and several results are available in the literature [9, 13, 22, 27].

Different procedures have been proposed along the years to obtain explicit expressions of Ω_k for any k in terms of commutators: recurrence relations [21], techniques based on binary trees [20], combinatorial techniques applied to iterated integrals [2, 26, 31], etc. The expressions thus obtained for Ω_k present however some limitations: they are not unique (due to the Jacobi identity and other identities appearing at higher orders) and very often not all the terms are independent. For certain applications it might be of some interest to get expressions similar to (5) for *any* given Ω_k, i.e., writing an arbitrary Ω_k as an *iterated integral* of (a linear combination of) *independent* nested commutators of A evaluated at different times. As far as we know, this has been carried out only up to $k = 6$ [22] and it is the purpose of this paper to provide a general expression for any $k \geqslant 1$, namely we will provide an explicit formula for Ω_k as an iterated integral of a linear combination of $(k-1)!$ right-nested independent commutators of A evaluated at different times. In doing so we will relate the Magnus expansion with the well known Malvenuto–Reutenauer Hopf algebra of permutations [18], thus providing a new illustration of this abstract algebraic structure.

2. The Magnus expansion in terms of iterated integrals

As in [2, 30] our starting point is to write the Magnus series (3) in terms of iterated integrals of A. This can be achieved by considering the Neumann (Dyson) series for the solution of (1),

$$Y(t) = I + \int_0^t A(s)\,ds + \int_0^t dt_1 \int_0^{t_1} dt_2\, A(t_1)A(t_2) + \cdots$$

or, in general,

$$Y(t) = I + \sum_{n=1}^{\infty} P_n(t) \tag{7}$$

with

$$P_n(t) = \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n\, A(t_1)A(t_2)\,\cdots\,A(t_n). \tag{8}$$

This is a convergent series for all t (if A is bounded), but, in contrast to the Magnus expansion, when truncated no longer preserves qualitative properties of the exact solution. In particular, if $A(t)$ is a skew-Hermitian operator, the approximation thus obtained is no longer unitary.

The Ω_k can in fact be expressed in terms of the iterated integrals (8) by taking logarithms in (3) and equating with (7),

$$\sum_{k=1}^{\infty} \Omega_k(t) = \log\left(I + \sum_{k=1}^{\infty} P_k(t)\right).$$

Then

$$\Omega_n = P_n - \sum_{j=2}^{n} \frac{(-1)^j}{j} R_n^{(j)}, \qquad n \geqslant 2, \tag{9}$$

where

$$R_n^{(j)} = \sum P_{i_1} P_{i_2} \cdots P_{i_j} \qquad (i_1 + \cdots + i_j = n)$$

and the sum extends over all $i_1, i_2, \ldots i_j$ such that $i_1 + i_2 + \cdots + i_j = n$ [12]. Thus, in particular, we get for the first terms

$$\Omega_1 = P_1$$
$$\Omega_2 = P_2 - \frac{1}{2}P_1^2$$
$$\Omega_3 = P_3 - \frac{1}{2}(P_1 P_2 + P_2 P_1) + \frac{1}{3}P_1^3$$
$$\Omega_4 = P_4 - \frac{1}{2}(P_1 P_3 + P_3 P_1 + P_2^2) + \frac{1}{3}(P_1^2 P_2 + P_1 P_2 P_1 + P_2 P_1^2) - \frac{1}{4}P_1^4. \tag{10}$$

Notice, however, that from Ω_2 on, these expressions are not yet written in terms of time-ordered integrals. To achieve this goal we have to express the products $P_{i_1} \cdots P_{i_j}$ appearing in (9) as iterated integrals. In this respect, it is useful to introduce the following notation:

$$A(i_1 i_2 \ldots i_n) \equiv \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n\, A(t_{i_1})A(t_{i_2}) \cdots A(t_{i_n}). \tag{11}$$

Observe that the order in the integration is fixed, whereas the ordering of the product appearing in the integrand is indicated by the sequence $i_1, i_2, \ldots i_n$. According with this notation, we have

$$A(1) = \int_0^t dt_1 A(t_1), \qquad A(12) = \int_0^t dt_1 \int_0^{t_1} dt_2\, A(t_1)A(t_2)$$
$$A(2341) = \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \int_0^{t_3} dt_4\, A(t_2)A(t_3)A(t_4)A(t_1)$$

etc, whereas (8) simply reads

$$P_n(t) = A(12 \ldots n).$$

Having established a one-to-one correspondence between iterated integrals and permutations via equation (11), it is possible to encode the products appearing in (9) also in terms of permutations. Thus, in particular,

$$\Omega_2 = A(12) - \frac{1}{2}A(1) \cdot A(1)$$
$$\Omega_3 = A(123) - \frac{1}{2}A(1) \cdot A(12) - \frac{1}{2}A(12) \cdot A(1) + \frac{1}{3}A(1) \cdot A(1) \cdot A(1).$$

According with Fubini's theorem,

$$\int_0^{\alpha} dy \int_y^{\alpha} f(x, y)\, dx = \int_0^{\alpha} dx \int_0^{x} f(x, y)\, dy, \tag{12}$$

we have $A(1) \cdot A(1) = A(12) + A(21)$, so that

$$\Omega_2 = A(12) - \frac{1}{2}(A(12) + A(21)) = \frac{1}{2}(A(12) - A(21)). \tag{13}$$

Analogously, using again (12) one has

$$A(1) \cdot A(12) = A(123) + A(213) + A(312)$$
$$A(12) \cdot A(1) = A(123) + A(132) + A(231)$$
$$A(1) \cdot A(1) \cdot A(1) = A(123) + A(132) + A(213) + A(231) + A(312) + A(321), \tag{14}$$

so that, by inserting (14) into the expression of Ω_3 given in (10), we arrive at

$$\Omega_3 = \frac{1}{3} A(123) - \frac{1}{6} A(132) - \frac{1}{6} A(213) - \frac{1}{6} A(231) - \frac{1}{6} A(312) + \frac{1}{3} A(321). \tag{15}$$

This procedure can be generalized to higher orders by realizing that any product of integrals encoded in terms of permutations appearing in Ω_k can be replaced by a sum of all possible permutations of time ordering consistent with whatever time ordering existed within the factors of the original product [15]. This is again a consequence of Fubini's theorem (12). Thus, $A(1) \cdot A(12)$ in equation (14) is the sum of all permutations of three elements such that the second index is always less than the third index. On the other hand, in $A(1) \cdot A(1) \cdot A(1)$ there is no special ordering, so that there is no preferential order for the decomposition (and thus all possible permutations have to be taken into account), whereas

$$A(1) \cdot A(123) = A(4123) + A(3124) + A(2134) + A(1234).$$

By applying this procedure to Ω_4 as given by (10) we get a linear combination with rational coefficients of all the $4! = 24$ permutations from the set $\{1, 2, 3, 4\}$. In general, we have for any $n \geqslant 2$,

$$\Omega_n(t) = \sum_{\sigma \in \mathfrak{S}_n} (-1)^{d_b} \frac{d_a! \, d_b!}{n!} A(\sigma), \tag{16}$$

where $\sigma \in \mathfrak{S}_n$ denotes a permutation of $\{1, 2, \ldots, n\}$, d_a is the number of *ascents* in σ, d_b is the number of *descents* and the sum is over the $n!$ permutations of the symmetric group $\mathfrak{S}_n$. We recall that σ has an ascent in i if $\sigma(i) < \sigma(i + 1), i = 1, \ldots, n - 1$ and it has a descent in i if $\sigma(i) > \sigma(i + 1)$. Here $(i_1 i_2 \ldots i_n) = (\sigma(1) \, \sigma(2) \, \ldots \, \sigma(n))$. Clearly $d_a + d_b = n - 1$ so that (16) can be written only in terms of either d_a or d_b. In this last case one has the alternative expression

$$\Omega_n(t) = \frac{1}{n} \sum_{\sigma \in \mathfrak{S}_n} (-1)^{d_b} \frac{1}{\binom{n-1}{d_b}} A(\sigma), \tag{17}$$

or more explicitly

$$\Omega(t) = \sum_{n=1}^{\infty} \frac{1}{n} \sum_{\sigma \in \mathfrak{S}_n} (-1)^{d_b} \frac{1}{\binom{n-1}{d_b}} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \, A(t_{\sigma(1)}) A(t_{\sigma(2)}) \cdots A(t_{\sigma(n)}). \tag{18}$$

This formula has been published a number of times in the literature, obtained by different techniques [2, 7, 26, 30]. If one is interested in writing Ω_n explicitly as an element in the Lie algebra generated by the family $A(t)$, the usual approach is then to apply the Dynkin–Specht–Wever theorem [11] to equation (17): the resulting expression is obtained by replacing

$$A(t_{\sigma(1)}) A(t_{\sigma(2)}) \cdots A(t_{\sigma(n)}) \quad \text{by} \quad \frac{1}{n}[A(t_{\sigma(1)}), [A(t_{\sigma(2)}), \cdots, [A(t_{\sigma(n-1)}), A(t_{\sigma(n)})] \cdots]]$$

in (17). In that case, though, not all the commutators appearing in the corresponding formula are linearly independent among each other, due to antisimmetry and the Jacobi identity. By contrast, in the formulation we propose all the terms are independent.

3. Iterated integrals and the Hopf algebra of permutations

The product $A(\sigma) \cdot A(\tau)$, with σ and τ two given permutations, that we introduced in the previous section just as a symbolic way of encoding the product of iterated integrals P_j, correspond in fact to a much deeper characterization of the set of permutations. This is in fact related with the Malvenuto–Reutenauer Hopf algebra of permutations, introduced and studied in [25, 28]. We next briefly recall the construction of this Hopf algebra. In doing so we follow the notation used originally in [25] for the product(s) and coproduct(s).

By following [4], let us denote by $\mathfrak{S}Sym$ the graded $\mathbb{Q}$-vector space with fundamental basis given by the disjoint union of the symmetric groups $\mathfrak{S}_n$ for all $n \geqslant 0$. In particular, $\mathfrak{S}_0 = \{()\}$ and the elements of $\mathfrak{S}_n$ are considered as words $\alpha = (a_1 a_2 \ldots a_n)$ on the alphabet $\{1, 2, \ldots, n\}$. In [25] two Hopf algebra structures on $\mathfrak{S}Sym$ are introduced as follows.

The product $*'$ of $\sigma \in \mathfrak{S}_k$ and $\tau \in \mathfrak{S}_\ell$ is defined by

$$\sigma *' \tau = \sigma \;\sqcup\!\sqcup\; \bar{\tau}, \tag{19}$$

where $\bar{\tau}$ is the word in $\{k + 1, \ldots, k + \ell\}$ is obtained by replacing in τ each i by $i + k$, and $\sqcup\!\sqcup$ denotes the usual shuffle product. Thus, for instance,

$$(1) *' (12) = (123) + (213) + (231)$$
$$(1) *' (21) = (132) + (312) + (321)$$
$$(12) *' (12) = (1234) + (1324) + (1342) + (3124) + (3142) + (3412).$$

Notice that the empty word (permutation) acts as the unit element. Given a word $\alpha = (a_1 a_2 \ldots a_m)$ without repeats over the alphabet $\{1, 2, \ldots, m\}$, its standardization $\mathrm{st}(\alpha)$ is the word obtained by applying to α the unique increasing bijection $\{a_1, \ldots, a_m\} \longrightarrow \{1, 2, \ldots, m\}$. For instance, $\mathrm{st}((324)) = (213)$ and $\mathrm{st}(( )) = ( )$. Then the coproduct δ' is defined as

$$\delta'(\alpha) = \sum_{\alpha = uv} \mathrm{st}(u) \otimes \mathrm{st}(v),$$

where the sum is over all concatenation factorizations of α. In particular,

$$\delta'((2431)) = \mathrm{st}(( )) \otimes \mathrm{st}((2431)) + \mathrm{st}((2)) \otimes \mathrm{st}((431)) + \mathrm{st}((24)) \otimes \mathrm{st}((31))$$
$$+ \mathrm{st}((243)) \otimes \mathrm{st}((1)) + \mathrm{st}((2431)) \otimes \mathrm{st}(( ))$$
$$= ( ) \otimes (2431) + (1) \otimes (321) + (12) \otimes (21) + (132) \otimes (1) + (2431) \otimes ( ).$$

With the counit defined by $\varepsilon(( )) = 1$ and $\varepsilon(\alpha) = 0$ if α has length $\geqslant 1$, $\mathfrak{S}Sym$ is a non-commutative and non-cocommutative Hopf algebra, graded by the length of permutations.

As a matter of fact, another product $*$ and another coproduct δ can be defined endowing $\mathfrak{S}Sym$ with a second Hopf algebra structure which happens to be isomorphic to the previous one. Given, as before, $\sigma \in \mathfrak{S}_k$ and $\tau \in \mathfrak{S}_\ell$,

$$\sigma * \tau = \sum uv, \tag{20}$$

where the sum is over all u, v such that $\mathrm{st}(u) = \sigma$, $\mathrm{st}(v) = \tau$ and the concatenated word uv is a permutation in $\mathfrak{S}_{k+\ell}$. Thus, for instance,

$$(1) * (12) = (123) + (213) + (312)$$
$$(1) * (21) = (132) + (231) + (321)$$
$$(12) * (12) = (1234) + (1324) + (1423) + (2314) + (2413) + (3412).$$

Denoting by α_B the word obtained from α by removing all letters that are not in B, the coproduct is defined as

$$\delta(\alpha) = \sum_{i=0}^{n} \alpha_{\{1,\ldots,i\}} \otimes \mathrm{st}(\alpha_{\{i+1,\ldots,n\}}).$$

For example,

$$\delta((2431)) = ( ) \otimes \mathrm{st}((2431)) + (1) \otimes \mathrm{st}((243)) + (21) \otimes \mathrm{st}((43))$$
$$+ (231) \otimes \mathrm{st}((4)) + (2431) \otimes \mathrm{st}(( ))$$
$$= ( ) \otimes (2431) + (1) \otimes (132) + (21) \otimes (21) + (231) \otimes (1) + (2431) \otimes ( ).$$

These two graded Hopf algebras on $\mathfrak{S}Sym$ are isomorphic and dual to each other (i.e., self-dual) with respect to the inner product $\langle , \rangle$ defined as [18, 28]

$$\langle \sigma, \tau \rangle = \begin{cases} 1 & \text{if } \sigma = \tau^{-1} \\ 0 & \text{otherwise} \end{cases}$$

Then, the existence of the antipode is automatic [18]. Moreover, the antipode has infinite order, as shown in [4], where explicit formulas have also been derived.

Furthermore, if $\theta : \mathfrak{S}Sym \longrightarrow \mathfrak{S}Sym$ denotes the linear involution that takes a permutation σ to its inverse, $\theta(\sigma) = \sigma^{-1}$, then these two Hopf algebras are conjugated by θ:

$$\sigma * \tau = \theta(\theta(\sigma) *' \theta(\tau)) \quad \text{and} \quad \delta(\sigma) = (\theta \otimes \theta)(\delta'(\theta(\sigma))). \tag{21}$$

We notice at once the connection between the product of iterated integrals arising from the application of Fubini's theorem (see e.g. (14)) and the product $*$ of permutations in the Hopf algebra $\mathfrak{S}Sym$ via the one-to-one correspondence between iterated integrals and permutations (11): it clearly holds that

$$A(\sigma) \cdot A(\tau) = A(\sigma * \tau). \tag{22}$$

Relation (22) can be found in reference [2], where the product $*$ is referred to as shuffle product of permutations.

One might ask what is the equivalent, at the level of iterated integrals, of the product $*'$ in $\mathfrak{S}Sym$. To this end, we remark that it is possible to define another one-to-one correspondence between iterated integrals and

permutations, in addition to (11). Specifically, let us denote

$$A'(i_1 i_2 \cdots i_n) \equiv \int_0^t dt_{i_1} \int_0^{t_{i_1}} dt_{i_2} \cdots \int_0^{t_{i_{n-1}}} dt_{i_n} A(t_1) A(t_2) \cdots A(t_n), \tag{23}$$

so that the indices of the permutation indicate the simplex in which the integration is carried out, whereas the order in the functions appearing in the integrand is fixed. Then, it is straightforward to verify that

$$A'(i_1 i_2 \cdots i_n) = A((i_1 i_2 \cdots i_n)^{-1}) = A(\theta(i_1 i_2 \cdots i_n)).$$

Thus, the product of iterated integrals of the form (23) corresponds precisely to the product $*'$ in $\mathfrak{S}Sym$, and the map θ relates both types of iterated integrals, i.e.,

$$A'(\sigma) \cdot A'(\tau) = A'(\sigma *' \tau). \tag{24}$$

4. Magnus series in terms of right-nested independent commutators

The algorithm based on the application of (9), the product of permutations $*$ and the relation (22) allows us to construct Ω_n in the Magnus series explicitly in terms of elements in $\mathfrak{S}Sym$ for any $n \geqslant 1$. We next show that, by appropriately manipulating the expression (17), it is possible to write Ω_n in such a way that only right-nested independent commutators are present.

To illustrate the procedure, consider again the expressions of Ω_2 and Ω_3 given by (13) and (15), respectively. It is clear that (13) already corresponds to the formula collected in (5) for Ω_2, or equivalently

$$\Omega_2(t) = -\frac{1}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 \, [A(t_2), A(t_1)],$$

whereas (15) can be written as

$$\Omega_3 = \frac{1}{6}(A(123) - A(213)) - \frac{1}{6}(A(231) - A(321)) - \frac{1}{6}(A(312) - A(321))$$
$$+ \frac{1}{6}(A(123) - A(132)),$$

i.e.,

$$\Omega_3 = \frac{1}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 [A(t_1), A(t_2)]A(t_3)$$
$$- \frac{1}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 [A(t_2), A(t_3)]A(t_1)$$
$$- \frac{1}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 A(t_3)[A(t_1), A(t_2)]$$
$$+ \frac{1}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 A(t_1)[A(t_2), A(t_3)],$$

whence the expression (6) is recovered. Alternatively, Jacobi identity allows us to write also

$$\Omega_3 = \frac{1}{3} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \, [A(t_3), [A(t_2), A(t_1)]]$$
$$- \frac{1}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \, [A(t_2), [A(t_3), A(t_1)]].$$

If we denote, in general,

$$A[i_1, i_2, \ldots, i_n] \equiv \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n [A(t_{i_1}), [A(t_{i_2}), \cdots [A(t_{i_{n-1}}), A(t_{i_n})] \cdots]]$$

then we can write in a more compact way

$$\Omega_2 = -\frac{1}{2} A[2, 1], \qquad\qquad \Omega_3 = \frac{1}{3} A[3, 2, 1] - \frac{1}{6} A[2, 3, 1].$$

For higher order terms the same strategy can be applied, namely we can expand (17) and then collect the resulting terms into multiple commutators, although the procedure is cumbersome for $n \geqslant 4$. We rely instead in results presented in [15] concerning the set of all $(N-1)$-fold commutators of N different (abstract) linear operators $O_1, O_2, \ldots, O_N$. Specifically, in the appendix of [15] it is shown that

(1) This set forms a vector space of dimension $(N-1)!$.

(2) A possible basis for this vector space is formed by right-nested commutators of the form

$$[O_m, [O_\ell, \ldots [O_k, O_j] \ldots]].$$

(3) In forming such a basis we can use only those right-nested commutators ending with a particular but otherwise arbitrary operator selected from the collection $O_1, O_2, \ldots, O_N$. If we choose this operator as O_1, then the basis is formed by the right-nested commutators of the form

$$[O_k, [O_j, \ldots [O_i, O_1] \ldots]],$$

where the indices $k, j, \ldots i$ are all possible permutations of $\{2, 3, \ldots N\}$ (clearly, $(N - 1)!$ permutations).

(4) Consider an expression which is known to be decomposable into a set of $(N - 1)$-fold commutators of N objects and suppose all the right-nested commutators ending with O_1 are used as a basis for the decomposition. Then, the coefficient of the right-nested commutator $[O_k, [O_j, \ldots [O_i, O_1] \ldots]]$ is the coefficient of the permutation $\alpha = (kj\ldots i1)$ in the original expression.

These results can be readily applied to the expression (17) for Ω_n by identifying $O_i = A(t_i)$. In particular, for Ω_3 a basis of right-nested commutators can be taken as $\{[A(t_3), [A(t_2), A(t_1)]], [A(t_2), [A(t_3), A(t_1)]]\}$, associated with the permutations (321) and (231), respectively. The coefficients of (3 2 1) and (2 3 1) in (15) are respectively $\frac{1}{3}$ and $-\frac{1}{6}$, and so

$$\Omega_3 = \frac{1}{3} A[3, 2, 1] - \frac{1}{6} A[2, 3, 1]$$

in accordance with the previous direct calculation.

Taking into account these considerations, we can write in general

$$\Omega_n(t) = \sum_\sigma (-1)^{d_b+1} \frac{d_a!(d_b + 1)!}{n!} A[\sigma(2), \sigma(3), \ldots, \sigma(n), 1], \tag{25}$$

where now the sum extends over the $(n - 1)!$ permutations σ of $\{2, 3, \ldots, n\}$ and d_a (respectively, d_b) is the number of ascents (respect., descents) of the permutation σ and thus $d_a + d_b = n - 2$. Notice that the total number of descents of the permutation $(\sigma(2)\ \sigma(3)\ \ldots\ \sigma(n)\ 1)$ is precisely $d_b + 1$. Alternatively,

$$\Omega_n(t) = \frac{1}{n} \sum_\sigma (-1)^{d_b+1} \frac{1}{\binom{n-1}{d_b+1}} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n$$
$$[A(t_{\sigma(2)}), [A(t_{\sigma(3)}) \cdots [A(t_{\sigma(n)}), A(t_1)] \cdots]]. \tag{26}$$

As an illustration, the expression of Ω_4 reads

$$\Omega_4 = -\frac{1}{4} A[4, 3, 2, 1] + \frac{1}{12} A[4, 2, 3, 1] + \frac{1}{12} A[3, 2, 4, 1]$$
$$+ \frac{1}{12} A[3, 4, 2, 1] + \frac{1}{12} A[2, 4, 3, 1] - \frac{1}{12} A[2, 3, 4, 1].$$

According with the preceding results, one could select any other $A(t_i)$ as the last operator (to the right) in the nested commutators, and so there are n different but equivalent expressions for Ω_n. In particular, if we take $O_1 \equiv A(t_n)$, then

$$\Omega_n(t) = \frac{1}{n} \sum_{\sigma \in \mathfrak{S}_{n-1}} (-1)^{d_b} \frac{1}{\binom{n-1}{d_b}} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n$$
$$[A(t_{\sigma(1)}), [A(t_{\sigma(2)}) \cdots [A(t_{\sigma(n-1)}), A(t_n)] \cdots]]. \tag{27}$$

In any case, these identities can be readily implemented in a computer algebra system to generate any order in the Magnus expansion.

5. Concluding remarks

The Magnus expansion is an extremely useful device when dealing with time-dependent linear differential equations of the form $Y' = A(t) Y$. It yields the solution of such equations in exponential form, the exponent defined as an infinite series whose terms can be constructed in a recursive way as multiple integrals of nested commutators of the operator $A(t)$ defining the differential equation. Given its ubiquitous nature and the wide range of applications in physics and mathematics, it is hardly surprising that along the years several authors have

proposed explicit formulas for the terms $\Omega_n(t)$ of the Magnus series. As a matter of fact, the same formulas can be found in various published references, independently obtained by different authors. Such expressions could be classified into two types: either Ω_n is written as a time-ordered integral of a sum of products of A evaluated at different times (as in [26]) or it is expressed as multiple integrals of a linear combination of $(n - 1)$-nested commutators [19]. Of course, as pointed out in section 2, by application of the Dynkin–Specht–Wever (DSW) theorem it is always possible to get an expression of the second type from the first approach. The drawback, though, is that there are many redundancies due to the Jacobi identity and other identities of commutators appearing at high orders.

By contrast, in the procedure we propose here no use is done of the DSW theorem from (18). Instead we apply the results obtained by Dragt & Forest in [15] to get a general expression for Ω_n as an iterated integral of a linear combination of $(n - 1)!$ right-nested independent commutators of A evaluated at different times. Other expressions of this type have been obtained up to Ω_6 containing less terms [22], although no general expression has been proposed.

When developing our procedure we have also established a remarkable connection of the Magnus expansion with the Malvenuto–Reutenauer Hopf algebra. This rather special Hopf algebra is non commutative, non cocommutative, free as an algebra, cofree as a coalgebra and self-dual [18]. We have seen that the products defining this structure admits a natural interpretation in terms of products of the iterated integrals appearing in the Magnus expansion, so this feature provides an additional, physical realization of the Hopf algebra of permutations.

Given the close connection between the Magnus expansion and the Baker–Campbell–Hausdorff (BCH) formula (see e.g. [30]), it is clear that the expression (27) can be used to get the homogeneous Lie polynomials $Z_m(X, Y)$ in the expansion

$$Z = \log(e^X\,e^Y) = X + Y + \sum_{m=2}^{\infty} Z_m(X, Y).$$

Proceeding in this way we recover the result obtained in [23], although the resulting commutators appearing in (27) are not all independent. An algorithm for expressing Z in terms of a basis of the free algebra generated by X and Y has been presented in [14].

Although here we have treated only linear differential equations, it is clear that the same approach can also be applied to nonautonomous nonlinear systems with only minimal changes [3, 30] and in fact to any problem where iterated integrals of the type considered in this work appear, such as the Wilcox expansion in quantum mechanics [32], chronological calculus in control theory [1], rough paths, etc.

Other issues remain of course to be analyzed in more detail, in particular the connection with other Hopf algebras closely related with the Malvenuto–Reutenauer Hopf algebra such as the Hopf algebra of heap-ordered trees [16], the role played by connected permutations [28] in our setting and the formulation at the level of the Hopf algebra of the results obtained by Dragt & Forest. This will be the subject of a forthcoming paper [5].

After the completion of this work, we have become aware that the authors of [6] independently have obtained expression (27) as a consequence of their treatment of the Euler idempotent based on the computation of a logarithm in a certain pre-Lie algebra of planar, binary, rooted trees.

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References

[1] Agrachev A A and Gamkrelidze R V 1979 The exponential representation of flows and the chronological calculus *Math. USSR-Sb.* **35** 727–85

[2] Agrachev A A and Gamkrelidze R V 1994 The shuffle product and symmetric groups *Differential equations, Dynamical Systems, and Control Science* ed K D Elworthy, W N Everitt and E B Lee (Marcel Dekker) 365–82

[3] Agrachev A A and Gamkrelidze R V 1994 Volterra series and permutation groups *J. Math. Sci.* **71** 2409–33

[4] Aguiar M and Sottile F 2005 Structure of the Malvenuto-Reutenauer Hopf algebra of permutations *Adv. Math.* **191** 225–75

[5] Arnal A, Casas F, Chiralt C and Murua A Work in progress

[6] Bandiera R and Schätz F 2017 Eulerian idempotent, pre-Li.e. logarithm and combinatorics of trees *Technical Report* arXiv:1702.08907

[7] Bialynicki-Birula I, Mielnik B and Plebański J 1969 Explicit solution of the continuous Baker-Campbell-Hausdorff problem and a new expression for the phase operator *Ann. Phys.* **51** 187–200

[8] Blanes S and Casas F 2016 *A Concise Introduction to Geometric Numerical Integration* (Boca Raton, FL: CRC Press)

[9] Blanes S, Casas F, Oteo J A and Ros J 1998 Magnus and Fer expansions for matrix differential equations: the convergence problem *J. Phys. A: Math. Gen.* **22** 259–68

[10] Blanes S, Casas F, Oteo J A and Ros J 2009 The Magnus expansion and some of its applications *Phys. Rep.* **470** 151–238

[11] Bonfiglioli A and Fulci R 2012 Topics in noncommutative algebra. the theorem of campbell, baker, hausdorff and dynkin *Lecture Notes in Mathematics* vol 2034 (Berlin: Springer)

[12] Burum D P 1981 Magnus expansion generator *Phys. Rev.* B **24** 3684–92

[13] Casas F 2007 Sufficient conditions for the convergence of the Magnus expansion *J. Phys. A: Math. Theor.* **40** 15001–17

[14] Casas F and Murua A 2009 An efficient algorithm for computing the Baker-Campbell-Hausdorff series and some of its applications *J. Math. Phys.* **50** 033513

[15] Dragt A J and Forest E 1983 Computation of nonlinear behavior of Hamiltonian systems using Lie algebraic methods *J. Math. Phys.* **24** 2734–44

[16] Foissy L and Unterberger J 2013 Ordered forests, permutations, and iterated integrals *Int. Math. Research Notices* **2013** 846–85

[17] Hairer E, Lubich C and Wanner G 2006 *Geometric Numerical Integration. Structure-Preserving algorithms for Ordinary Differential equations* 2nd edn (Berlin: Springer)

[18] Hazewinkel M, Gubareni N and Kirichenko V V 2010 *Algebras, Rings and Modules. Lie Algebras and Hopf Algebras* (Providence RI: AMS)

[19] Iserles A, Munthe-Kaas H Z, Nørsett S P and Zanna A 2000 Lie-group methods *Acta Numerica* **9** 215–365

[20] Iserles A and S P Nørsett 1999 On the solution of linear differential equations in Li e groups *Phil. Trans. Royal Soc.* A **357** 983–1019

[21] Klarsfeld S and Oteo J A 1989 Recursive generation of higher-order terms in the Magnus expansion *Phys. Rev.* A **39** 3270–3

[22] Lakos G 2017 Convergence estimates for the Magnus expansion *Technical Report* arXiv:1709.01791

[23] Loday J-L 1994 Série de Hausdorff, idempotents Eulériens et algèbres de Hopf *Expo. Math.* **12** 165–78

[24] Magnus W 1954 On the exponential solution of differential equations for a linear operator *Comm. Pure and Appl. Math.* **VII** 649–73

[25] Malvenuto C and Reutenauer C 1995 Duality between quasi-symmetric functions and the Solomon descent algebra *J. Algebra* **177** 967–82

[26] Mielnik B and Plebański J 1970 Combinatorial approach to Baker-Campbell-Hausdorff exponents *Ann. Inst. Henri Poincaré* **XII** 215–54

[27] Moan P C and Niesen J 2008 Convergence of the Magnus series *Found. Comput. Math.* **8** 291–301

[28] Poirier S and Reutenauer C 1995 Algèbres de Hopf de tableaux *Ann. Sci. Math. Québec* **19** 79–90

[29] Prato D and Lamberti P 1997 A note on Magnus formula *J. Chem. Phys.* **106** 4640–3

[30] Strichartz R S 1987 The Campbell-Baker-Hausdorff-Dynkin formula and solutions of differential equations *J. Funct. Anal.* **72** 320–45

[31] Vinokurov V A 1992 Logarithm of the solution of a linear differential equation, the Hausdorff formula and conservation laws *Soviet Math. Dokl.* **44** 200–5

[32] Wilcox R M 1967 Exponential operators and parameter differentiation in quantum physics *J. Math. Phys.* **8** 962–82